

Theoretical Investigations of 2-Vinylpyridine Stereoselective Polymerization Catalyzed by Cationic Yttrium Complexes with Different Ancillary Ligands

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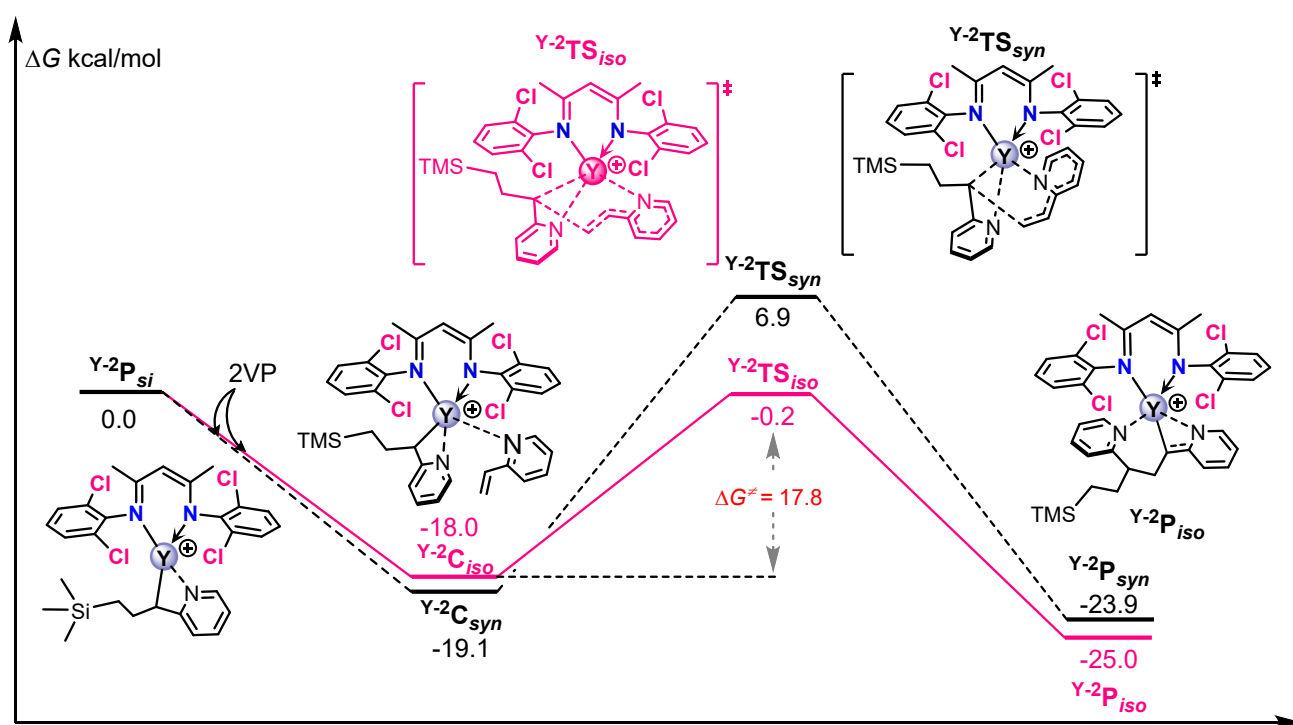


Figure S1. Calculated energy profiles for 2VP insertion into Y-2 complex (isotacticity). The isotactic path is in pink and the syndiotactic one is in black (energies in kcal/mol).

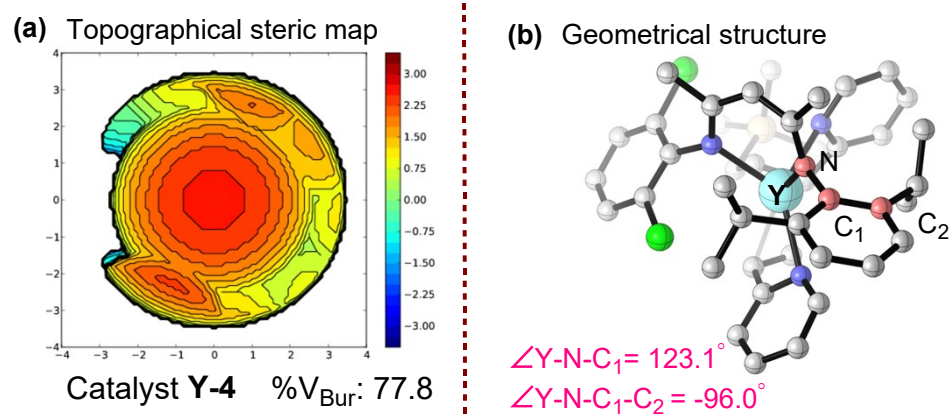


Figure S2. (a) Topographical steric maps of catalyst **Y-4** (b) Geometrical structures of $Y-4TS_{iso}$.